LANSCE DIVISION RESEARCH REVIEW

The Deformation Mechanism of a Uranium 6 weight % Niobium Alloy

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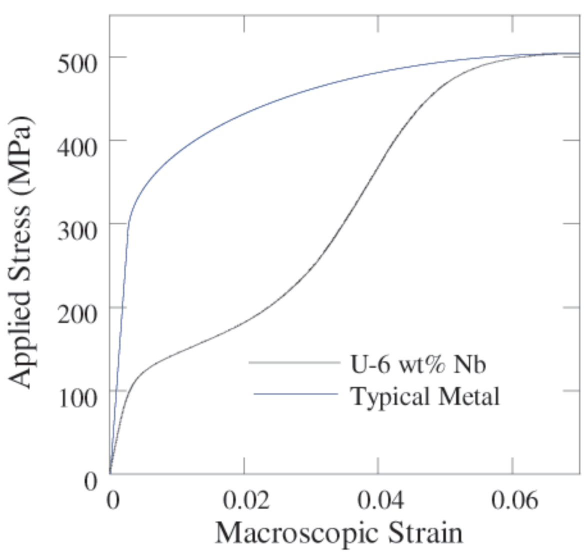
This work was directed at the determination of the deformation mechanisms of Uranium 6 weight % Niobium (15.4 atomic %) an alloy of interest to the Stockpile Stewardship program at LANL. Its deformation mechanisms are not, to date, well understood, and attempts at modeling the mechanical behavior of the alloy using existing constitutive models have been unsuccessful. In order to successfully model the behavior of U6Nb and advance the SBSS mission, it is necessary to develop a solid physical understanding of the deformation mechanisms of this material.

U6Nb has a monoclinic structure derived from the orthorhombic structure of pure Uranium. The structure may be pictured as a rectangular parallelepiped, with one angle, that between the a and b parameters, increased from 90° to 92.3°. The difficulty in modeling U6Nb lies in its atypical response to mechanical stress, shown in the form of a stress-strain curve in Figure 1. For comparison, a schematic stress-strain curve of a typical metal with similar mechanical properties is also depicted in Figure 1.



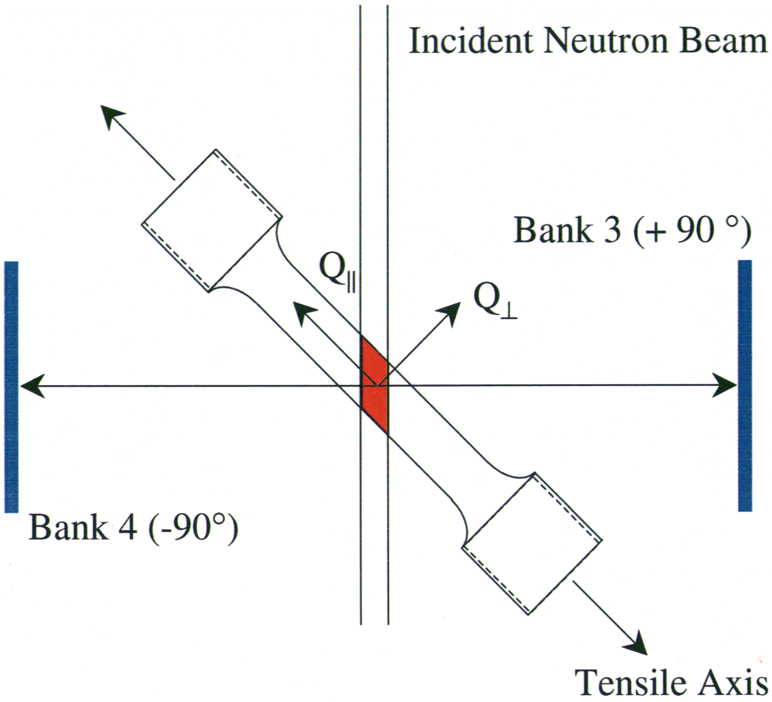
▲ ***Fig. 1.*** *Stress Strain Curve of U6Nb along with schematic of that of a typical metal.*

A typical metal will elongate linearly and elastically with applied stress until the yield point, sy, is reached. Beyond this point the material work-hardens and lengthens much more rapidly with stress (plastic flow) until, finally, the material ruptures. The plastic behavior, generally referred to as slip, is well understood and is captured by the popular MTS and PTW computer models currently in use.

The U6Nb alloy deforms in a linear elastic manner with applied stresses to roughly 125 MPa. Above 125 MPa between strains of 0.3 and 3%; however, there is a stress plateau in the stress/strain curve, after which the work-hardening again increases. Finally, above 3% strain the material flows in a way reminiscent of simple plasticity. Upon closer inspection, we find a maximum in the stress-strain curve at ~ 700 MPa, which Vandermeer associates with the start of irreversible plastic flow [1]. Below 700 MPa, or roughly 7% strain, the imparted strain is, to a large degree (~ 98%), recoverable on heating; that is, the material exhibits the shape memory effect (SME).

Figure 2 shows a schematic of the stress rig on the Neutron Powder Diffractometer (NPD) at the Lujan Center [2]. The incident white neutron beam impinges on the sample and is scattered into the detector banks situated at ± 90° relative to the inci dent beam. Data is recorded with diffraction vector, Q, parallel (bank 4) and perpendicular (bank 3) to the applied load simultaneously. From the schematic it can be seen that bank 4 (3) records information about the lattice spacing of grains with crystal planes whose normals are oriented parallel (perpen dicular) to the axis of the applied load. By applying stress to the sample in-situ and utilizing the lattice spacing as a strain gauge, we can monitor the mechanical response of the material to applied stress. For instance, the lattice parameters of simple materials are found to increase linearly with applied tension while in the elastic regime.

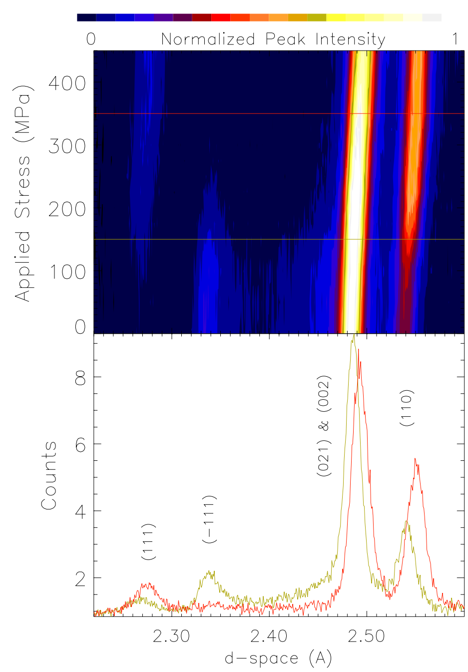
There are three recognized possible mechanisms for the anomalous stress-strain behavior of U6Nb, each easily identifiable by in-situ neutron diffraction measurements. In the case of a system in which slip is the active deformation mechanism, a saturation of the lattice strains is expected. Once slip begins, the



▲ *Fig. 2. Schematic of the NPD.*Center

system ceases to store elastic energy in the expan sion of the lattice. Twinning, which is a local reorie tation of the crystal lattice, is a second possible deformation mechanism that also has an identifable experimental signature. If twinning is active, one or more of the lattice parameters will undergo a strain reversal; that is, the elastic lattice strain, monitored by neutron diffraction, will relax with continued applied tension. Also, because twinning involves a lattice reorientation, it will be manifested by a marked variation (increase/decrease) of the sin gle-peak diffraction intensities. Finally, stress relax ation may occur through a stress-induced phase transformation. In this case, the zero_----stress dif fraction pattern will be replaced, on transformation, by a different diffraction pattern that reflects the symmetry of the new crystal structure.

Figure 3 shows a representative diffraction pattern taken at a load of 150 MPa, as well as a contour plot of the diffraction intensity versus d-space and applied load. The shift of the peaks to higher d-spacing with increased load is due to the applied tension. It is evident that the intensity of the (110) and (111) peaks increases significantly with increas ing load between 125 and 300 MPa, while the inten sities of the (-111) and (021) peaks decrease. This coincides with the low-stress-flow region of the stress/strain curve and is a strong indication that twinning is active in this region. Note that no new

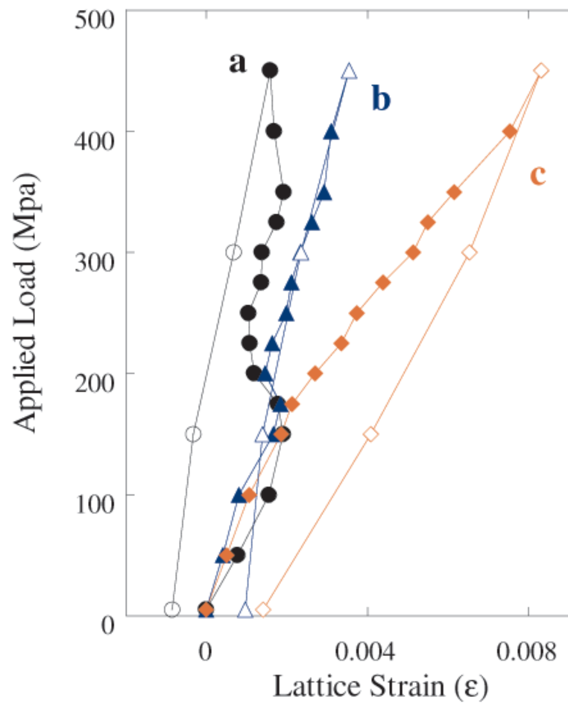


▲ *Fig. 3. Contour plot of diffraction intensity vs. d-spacing and applied load. The lower section shows cuts through the contour plot at applied loads of 150 (green) and 350 MPa (red). Note the shift of the diffraction peaks with load as well as the changing intensities.*

diffraction peaks appear, ruling out the possibility of a stress-induced phase transition in this region.

Figure 4 shows the behavior of the a, b, and c lattice parameters derived by Rietveld refinements [3] of diffraction patterns recorded in detector bank 4 as a function of applied load. Figure 4 shows the behav ior of the lattice spacings of grains oriented with crystal planes whose normals are parallel to the ten sile axis. Both the a and b lattice parameters under go strain reversals at 150 MPa, again in the low stress flow region. This is further confirmation of the identification of the deformation mechanism with twinning.

The positive identification of the deformation mech anism of U6Nb is of primary importance to MST Division as well as to X Division in their efforts to accurately access the safety and reliability of the aging stockpile. Having the correct physical under standing of the constitutive behavior will allow com puter modelers to develop accurate models of the mechanical properties of U6Nb for implementation into predictive codes. The deformation of U6Nb is still a work in progress, however. For twinning, it entails determining the twin plane(s) as well as the resolved shear stress at which twinning becomes active. We are presently analyzing the data already collected in order to accomplish this. Also, it will be necessary to study the material in compression as it is likely that the twin plane will be altered from the case of tension. Finally, the SME, which refers to the ability of the material to recover strains after unload ing and heating to moderate temperatures, observed in U6Nb, is of academic interest. While SME has been recognized in U6Nb since 1978 [4], structural studies of the mechanism of shape recovery are lack ing. We plan to do further neutron diffraction stud- ies of U6Nb at high temperatures to fill this void.



▲ ***Fig 4.*** *Applied load vs. lattice strain, closed (open) symbols represent data taken on loading (unloading). The strain reversal of the a and b parameters is a manifestation of twinning.*

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